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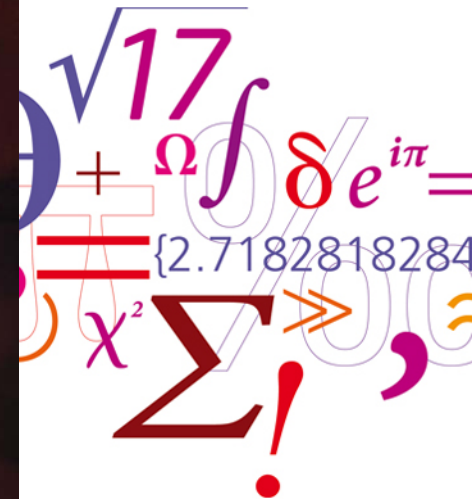
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High-resolution spectroscopy of gases at elevated temperatures

Alexander Fateev and Sønnik Clausen

Optical Diagnostics Group,

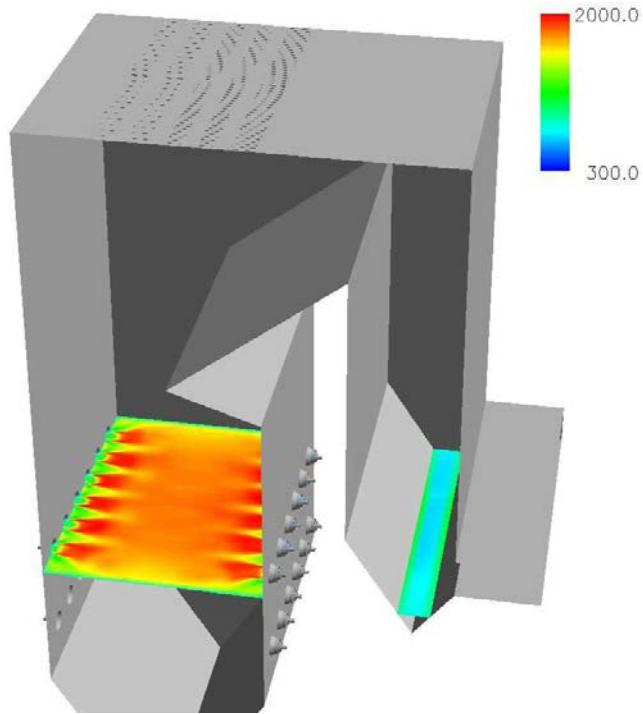
DTU Chemical Engineering, Frederiksborgvej 399, Roskilde, DK-4000, Denmark



Outline

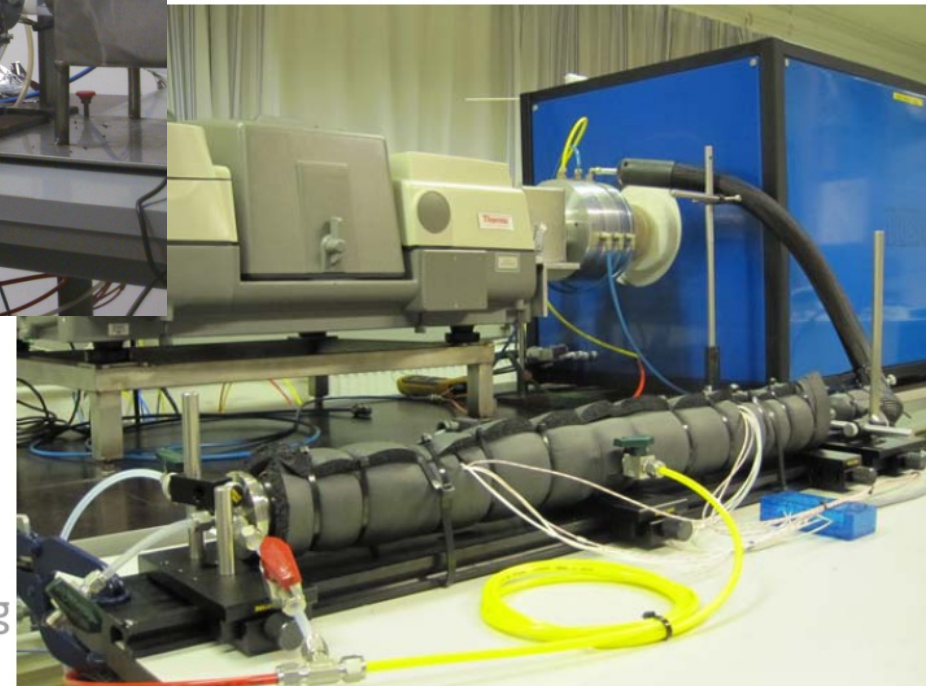
- Large scale measurements: why?
- Basic research: how it's made
- High resolution spectroscopy in flow gas cells: CO₂(IR), SO₂(one molecule: two applications) and Phenol(UV)
- SO₃ project: the story
- Conclusions

Combustion: flames and hot flue gases



Basic research

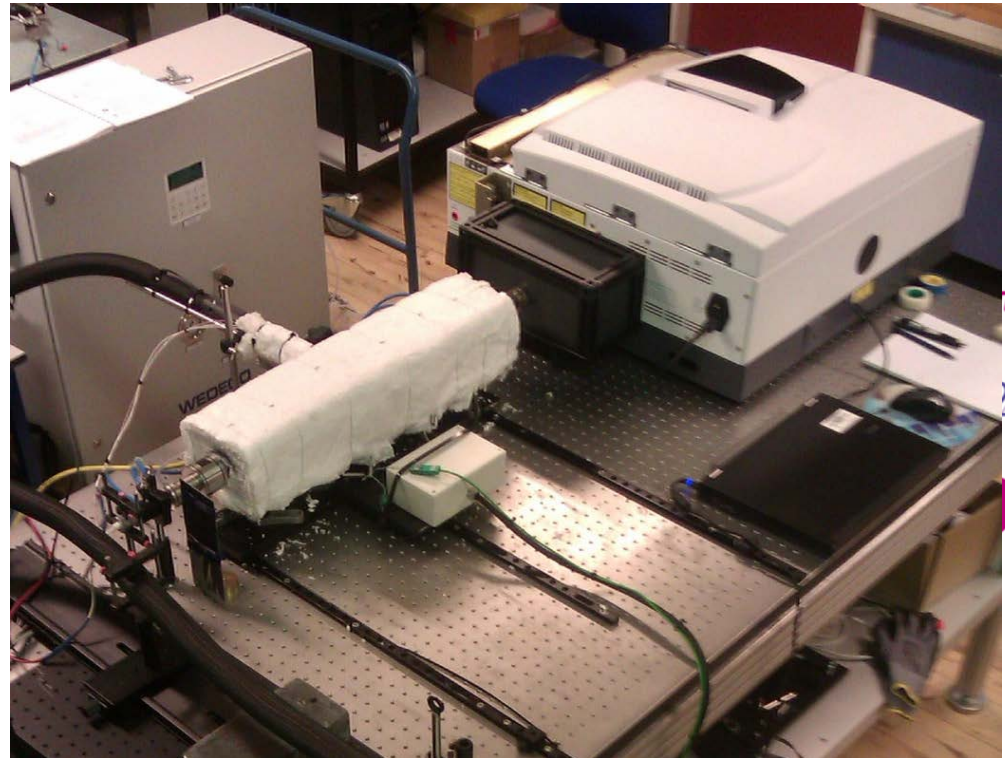
- focus on optical properties (TRS, ABS) of gases at temperatures up to 1600C;
- validation/building databases (e.g. HITRAN/HITEMP/CDSD...);
- various hot gas cells with highly-uniform temperature profiles ($\pm 0.5^\circ\text{C}$).



Basic research

high-resolution spectroscopy ($0.125\text{ cm}^{-1}/0.016\text{ nm}$) of “major” and “minor” (or trace) gases :

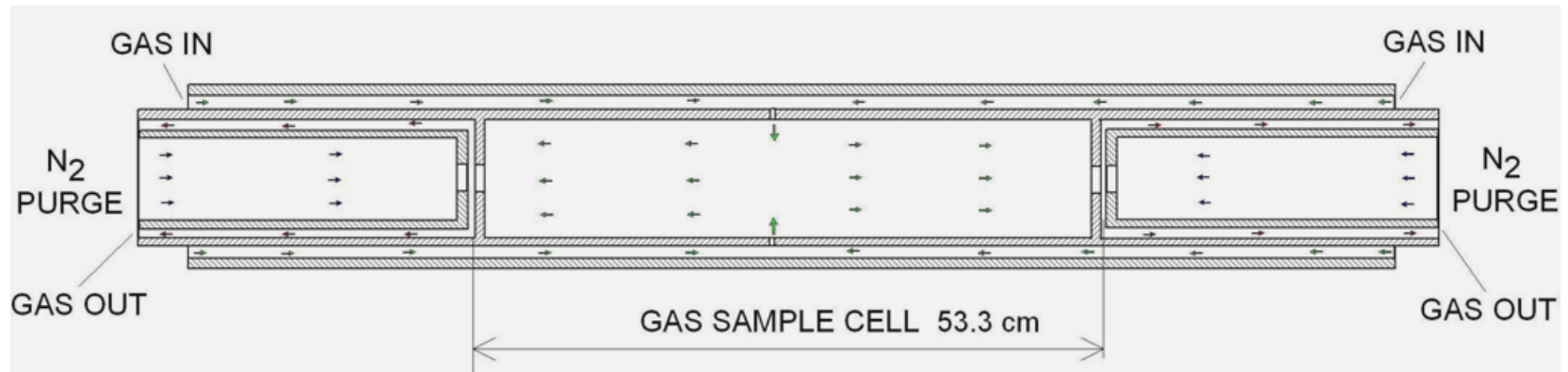
- CO_2
- H_2O
- SO_2
- NH_3
- SO_3 , H_2S , OCS
- HCL , KCl , CH_3Cl
- PAH's,
- etc;



Experimental set up: flow gas cell



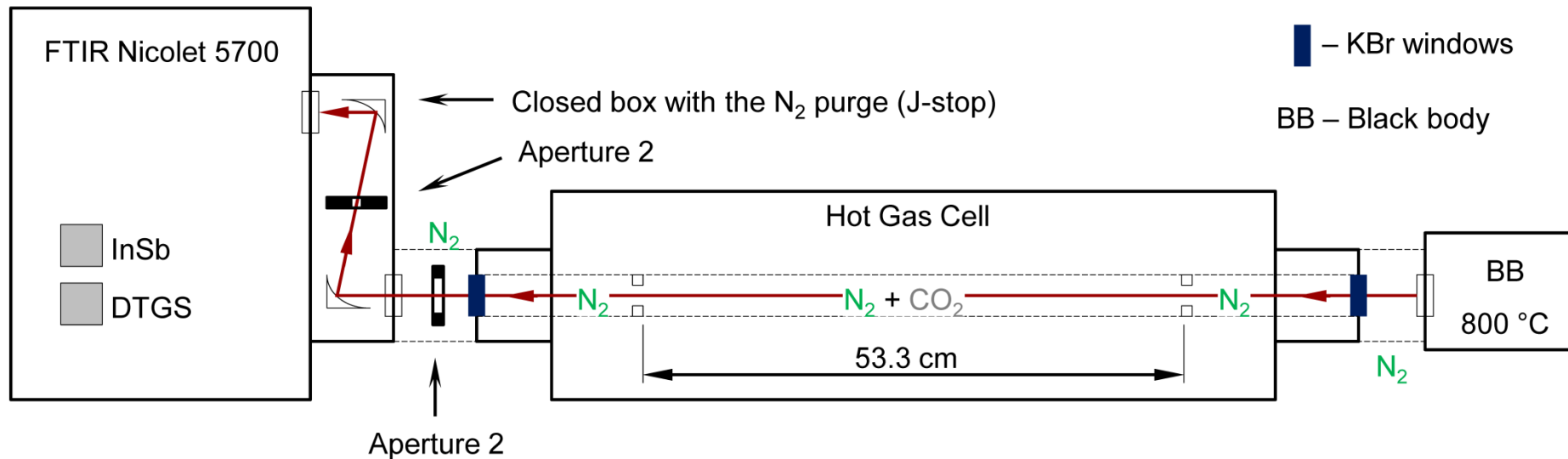
- 3-zones gas cell;
- Non-windows;
- Highly-stable uniform T-profile ($\pm 0.5^\circ\text{C}$);
- $T_{\text{max}} 1600^\circ\text{C}$
- $L = 53.3 \text{ cm}$
- $P = 1 \text{ bar}$



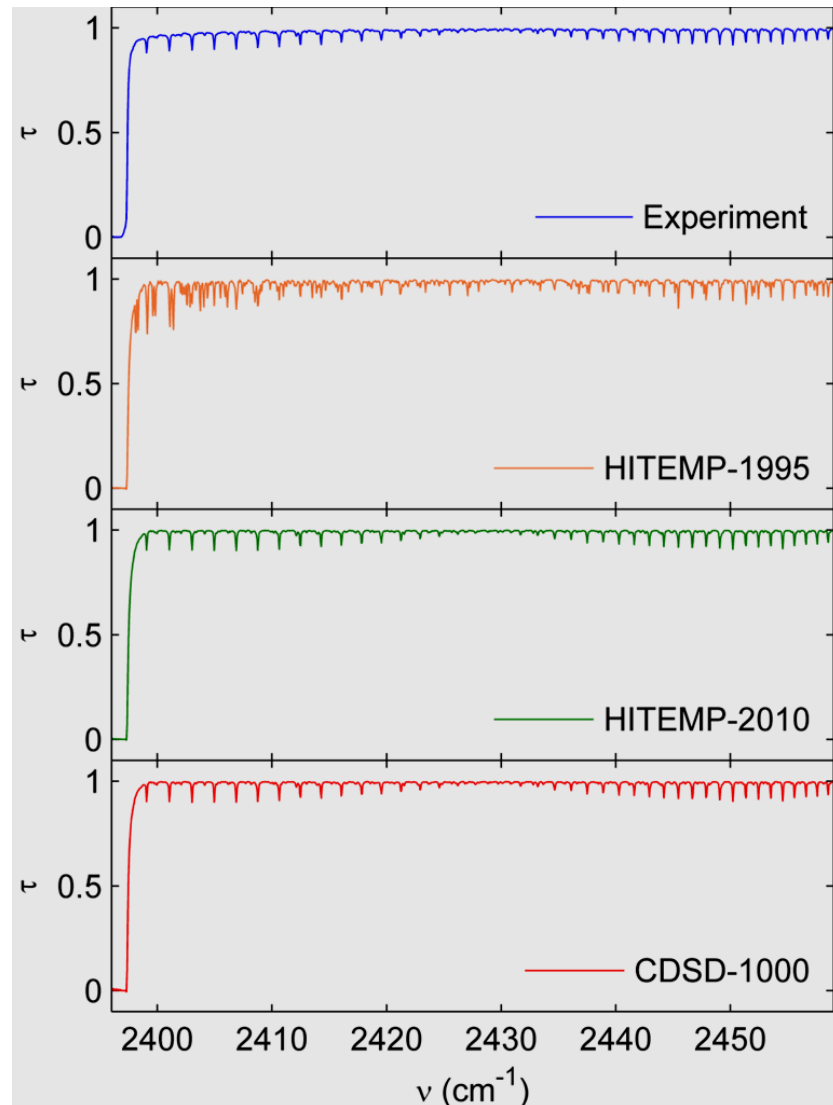
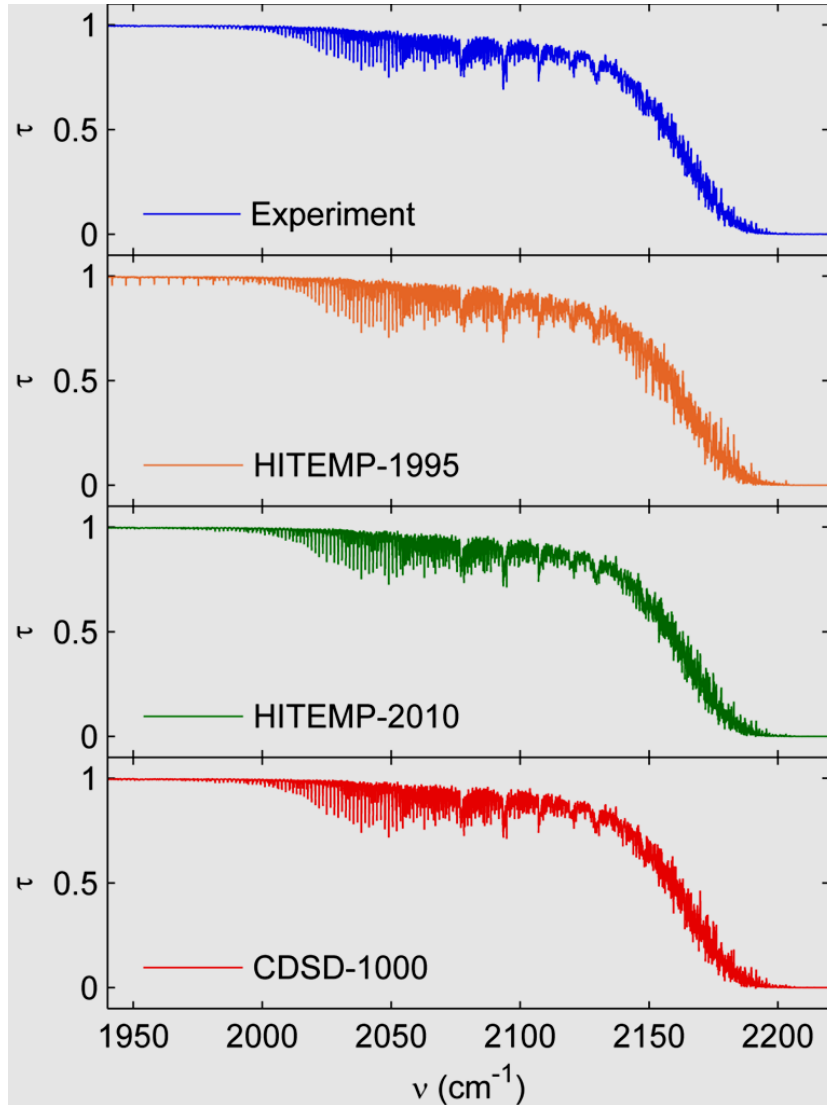
Experimental set up: gas cell + FTIR spectrometer

Includes:

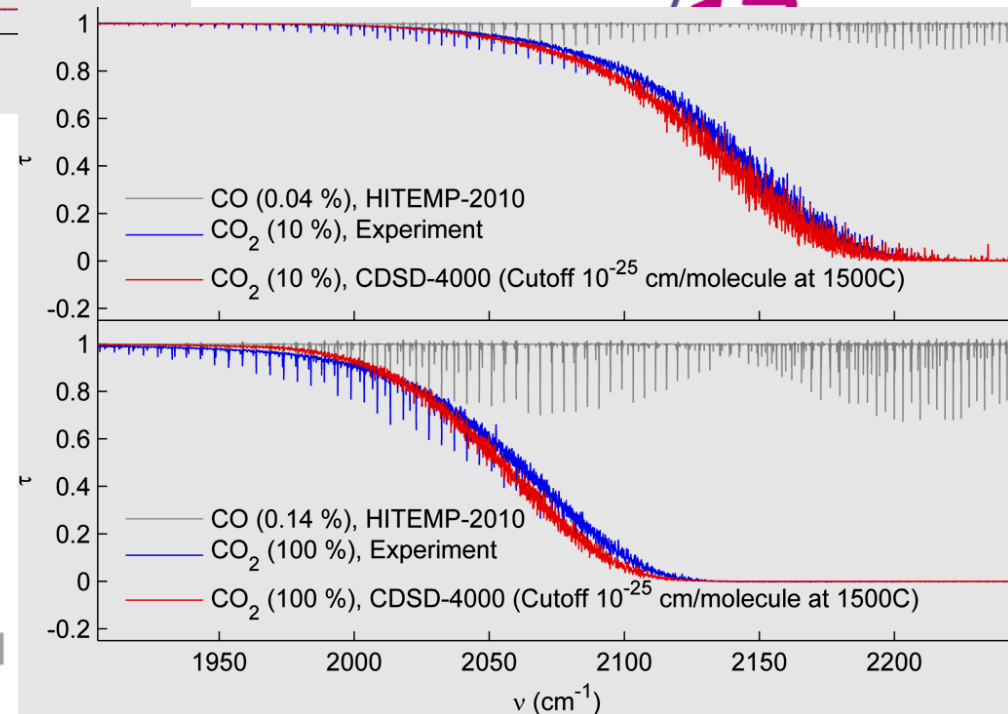
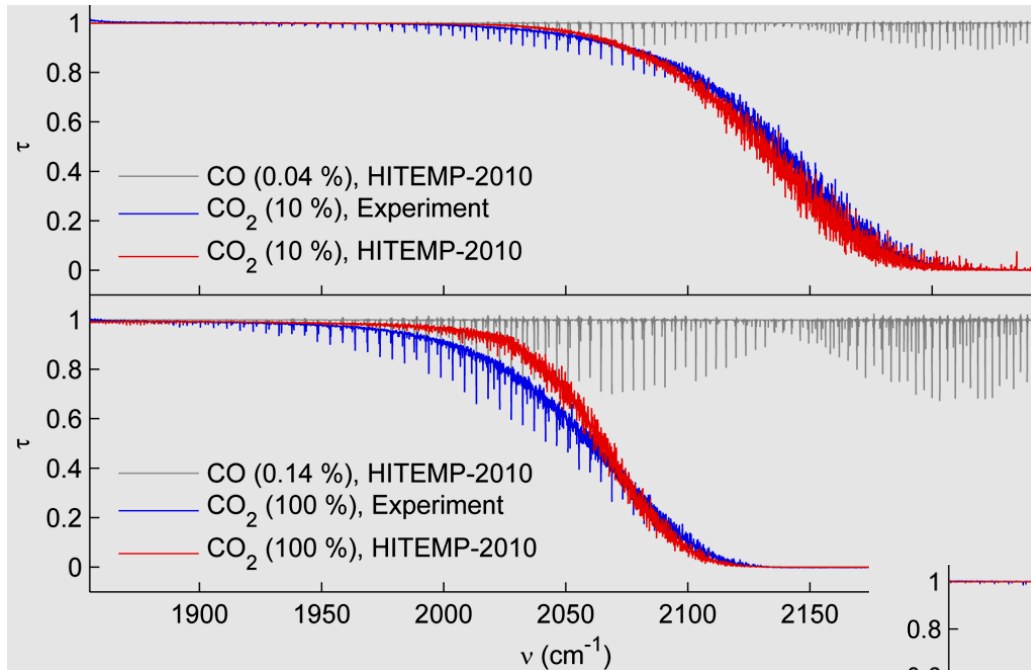
- a gas cell;
- a high-resolution FTIR spectrometer (Nicolet or Agilent);
- a light source (BB).



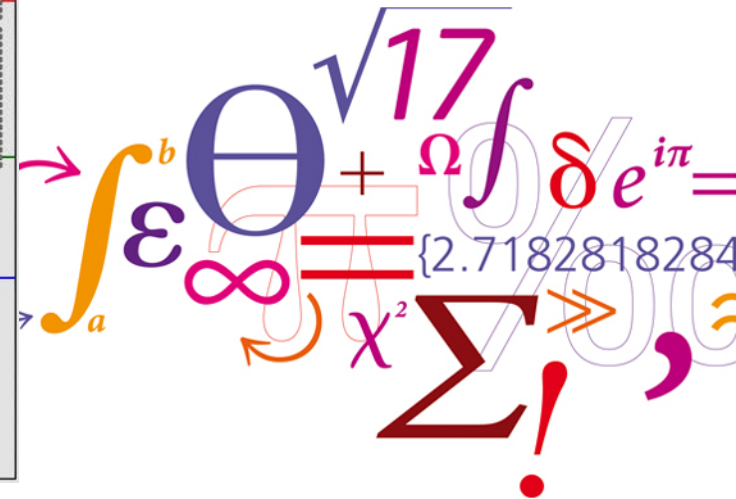
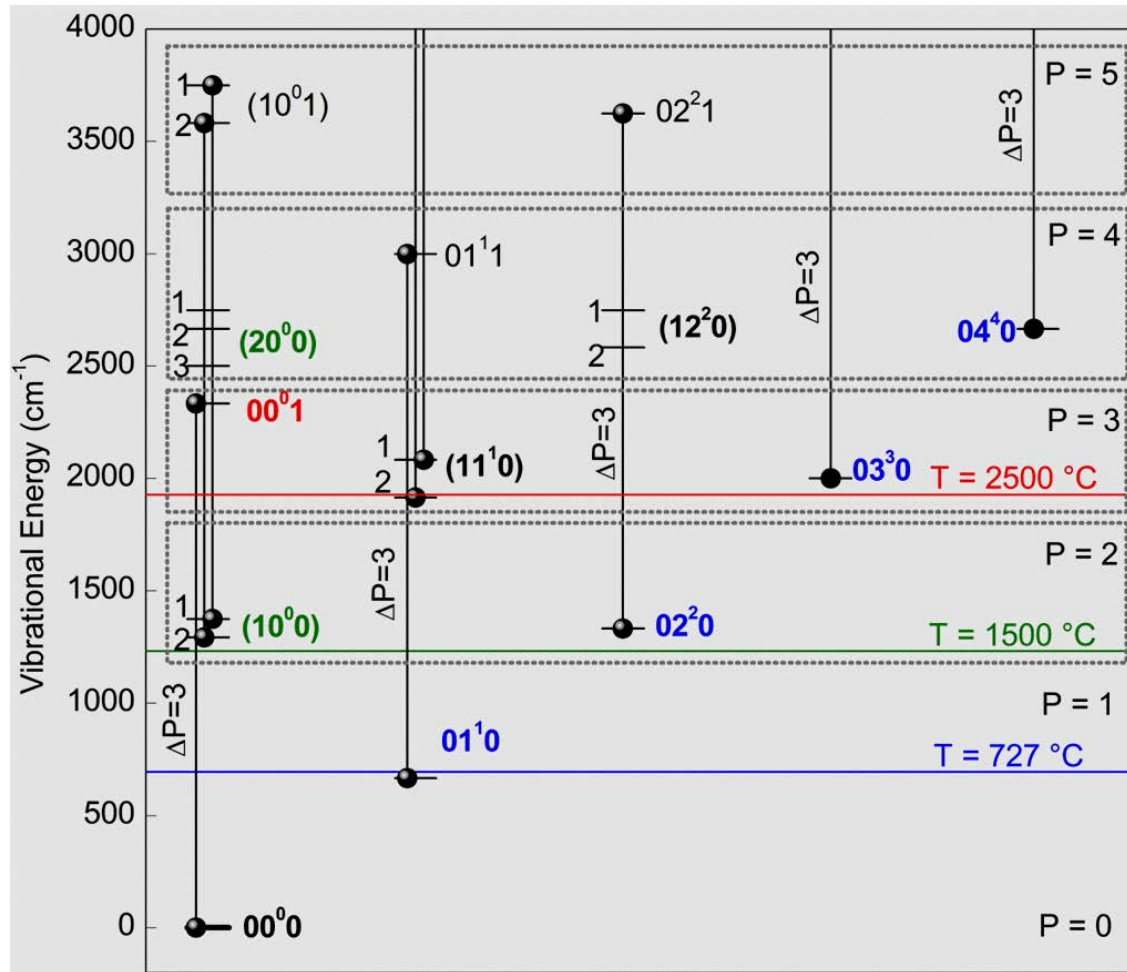
CO2 transmission spectra: 727C



CO₂ transmission spectra: 1500C



CO₂ quasicontinuum at 1500C



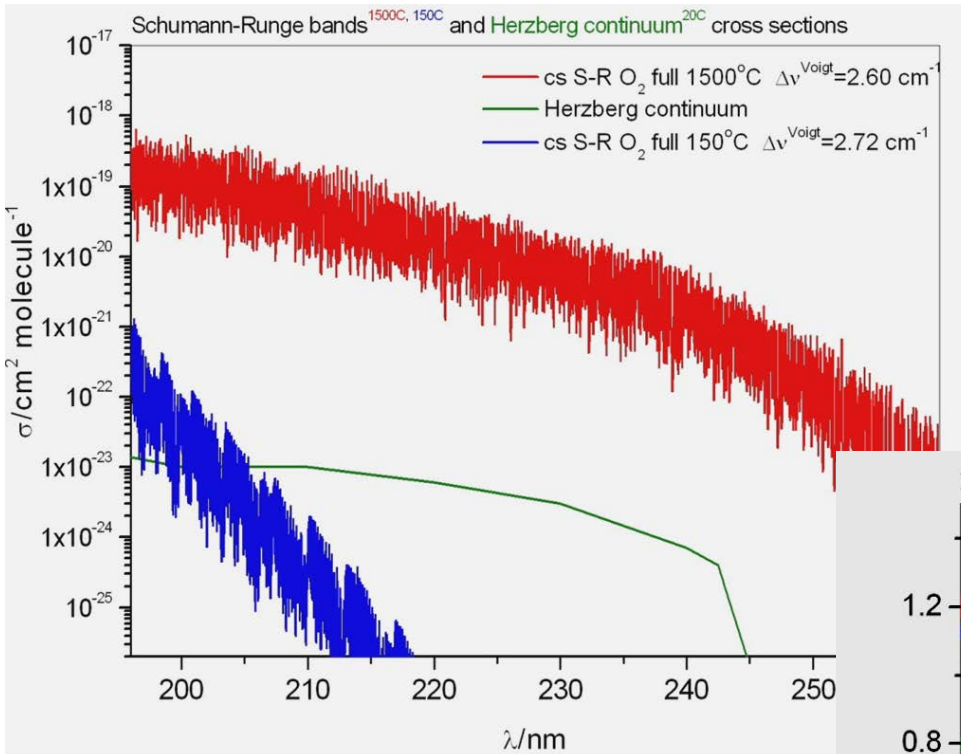
Details: JQSRT in press:

<http://dx.doi.org/10.1016/j.jqsrt.2012.07.015>

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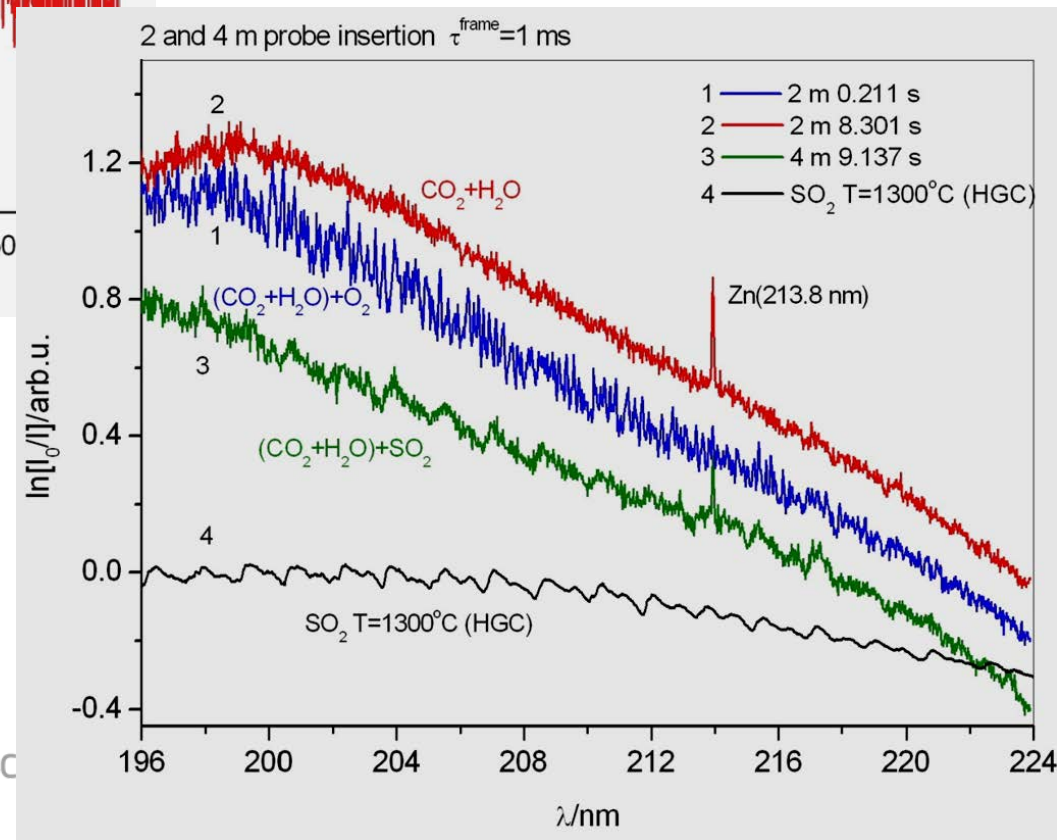
Department of Chemical and Biochemical Engineering

SO₂ spectroscopy: why?

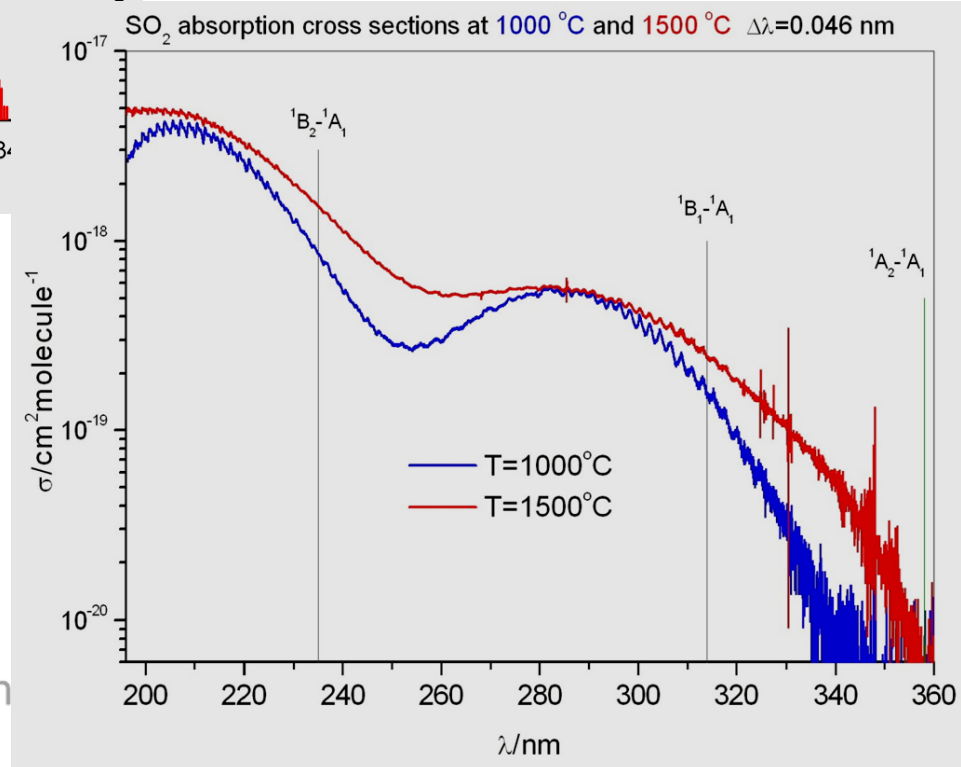
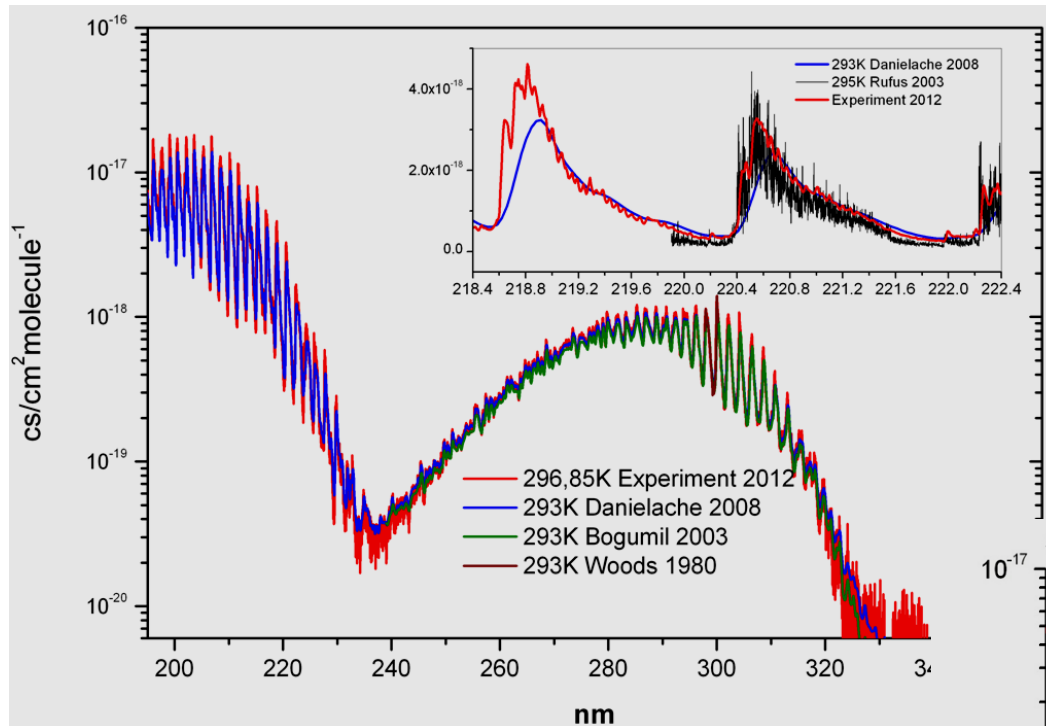


O₂ in turbulent flames:

- flame mapping
- mixing: combustion efficiency
- NO_x chemistry
- fast (few ms) measurements

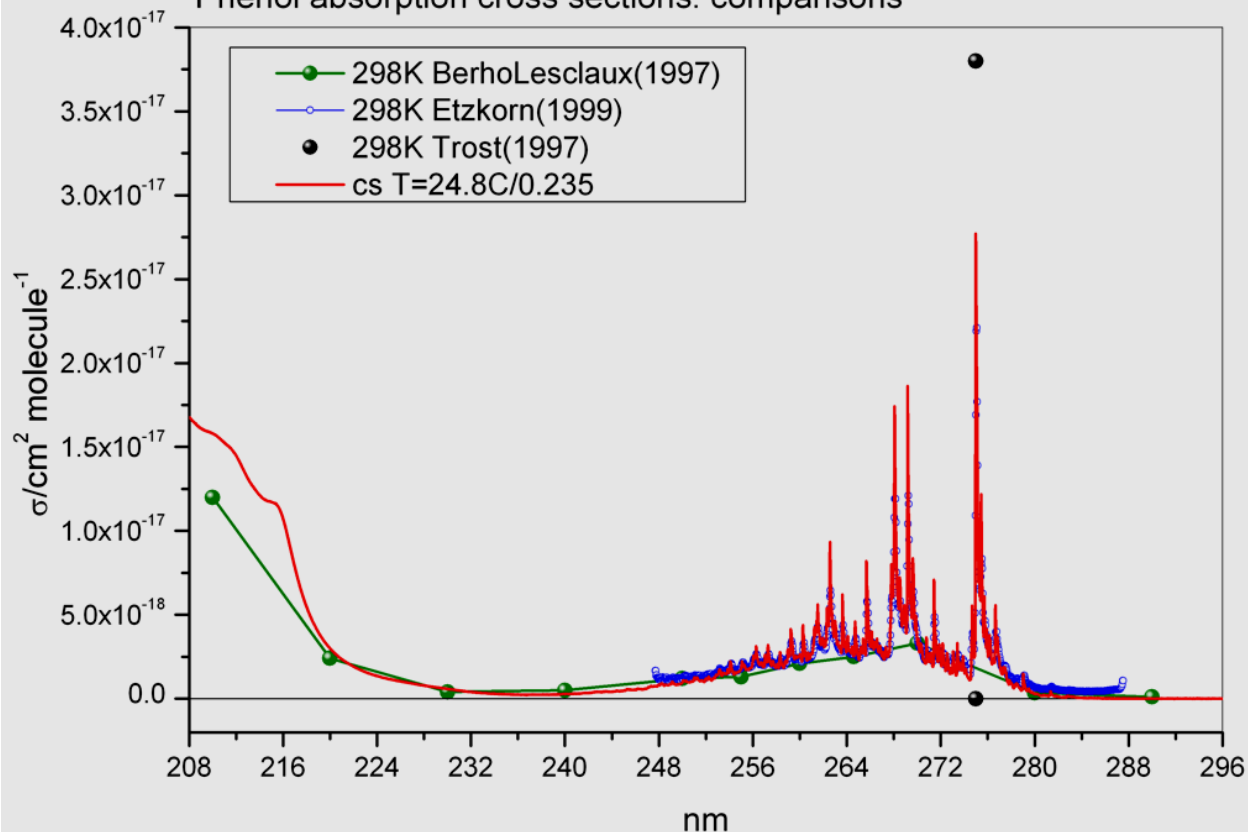


SO₂ spectroscopy: from validation to new data sets



Phenol spectroscopy: comparisons

Phenol absorption cross sections: comparisons

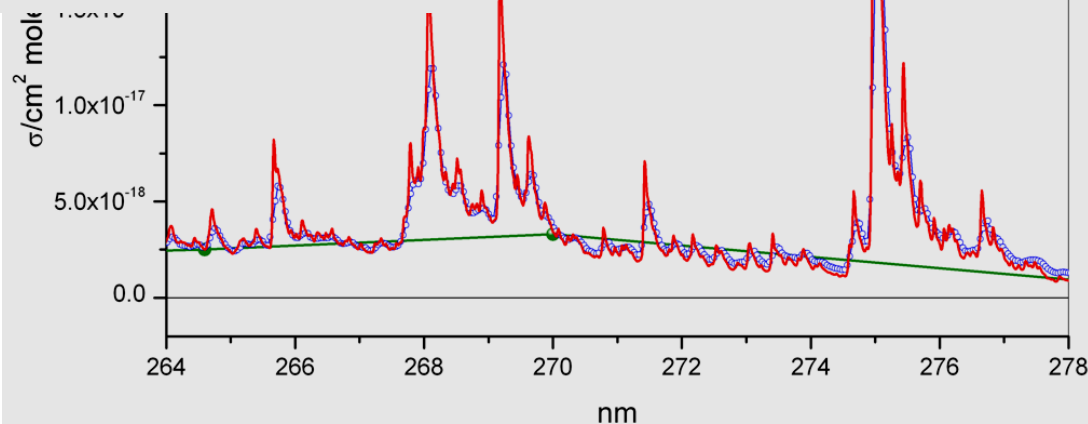


Phenol: solid to gas

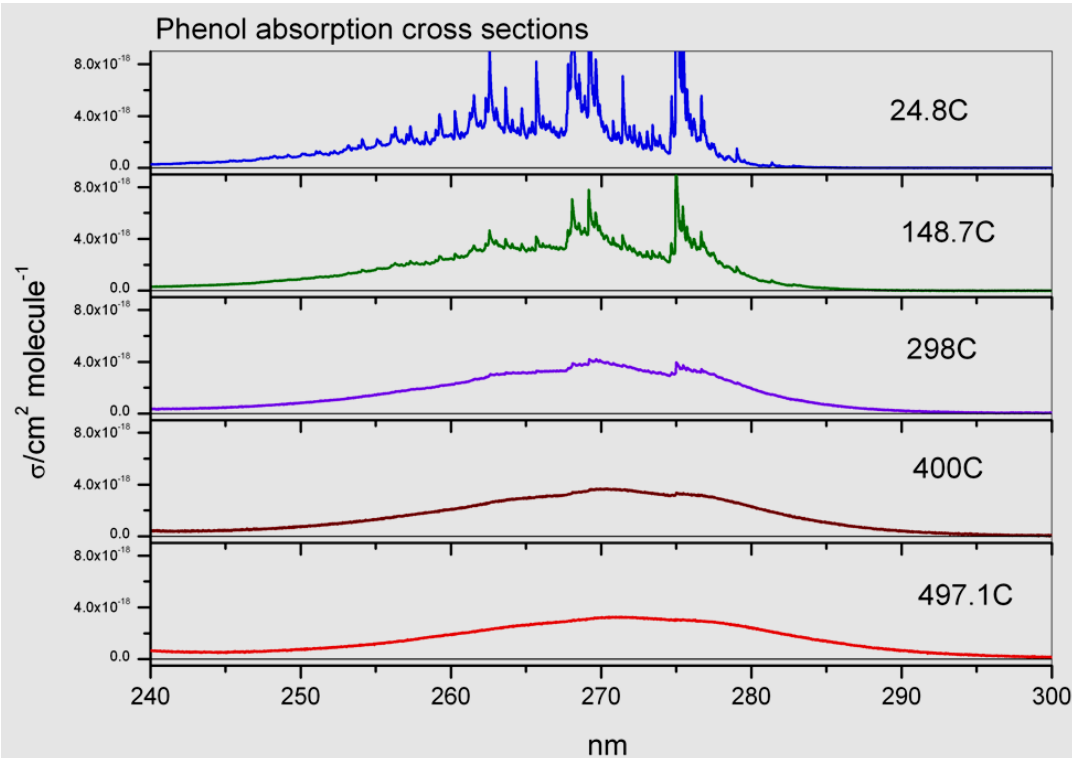
UV + GC/MS spectroscopy

sections: comparisons

claux(1997)
999)
35



Phenol spectroscopy: temperature effects in LT-CFB gasification



- Producer gas:
 - corrosion (boilers)
 - reduced gas quality (fuel cells, gas grids)
- Phenol – major trace gas from PAH's in producer gas (LT-CFB process);
- T_{gas} about 550C;

See more:

<http://www.dongenergy.com/pyroneer/Pages/index.aspx>

DTU Chemical Engineering
Department of Chemical and Biochemical

Pyroneer

A new Gasolution
- Biomass Gasification

Low Temperature
Gasification



Currently a 6MW demonstration plant is

LT-CFB



Gasification is a method for producing clean fuels from waste biomass and therefore has the potential to play a vast

Fuel and ash
partnerships



DONG Energy will supply future

6MW Project Status



Keep up with the status of our 6MW demonstration plant

SO3 project: industry and university

Facts:

- Coal air combustion: SO₂(300ppm) and SO₃(5ppm) (blue smog);
- Large power plants: SCR units (NO_x reduction) with NH₃ injection;
- Global warming: operation at lower loads;
- Lower loads: lower gas temperatures at SCR units;
- By law: not allowed to turn off NH₃ injection system.

Problems:

- Non optimal NH₃ consumption;
- At lower T: H₂SO₄ formation which causes ammonia sulfate and ammonia bisulfate formation;

Consequences:

corrosion in ducts and plugging/damage of SCR elements.

costs: entire incidental costs a five day unit outage for SCR work could cost more than **\$1 m** for a 500 MW unit

Goal:

to develop an optical method for SO₃ *in situ* measurements.

SO3 project: industry and university

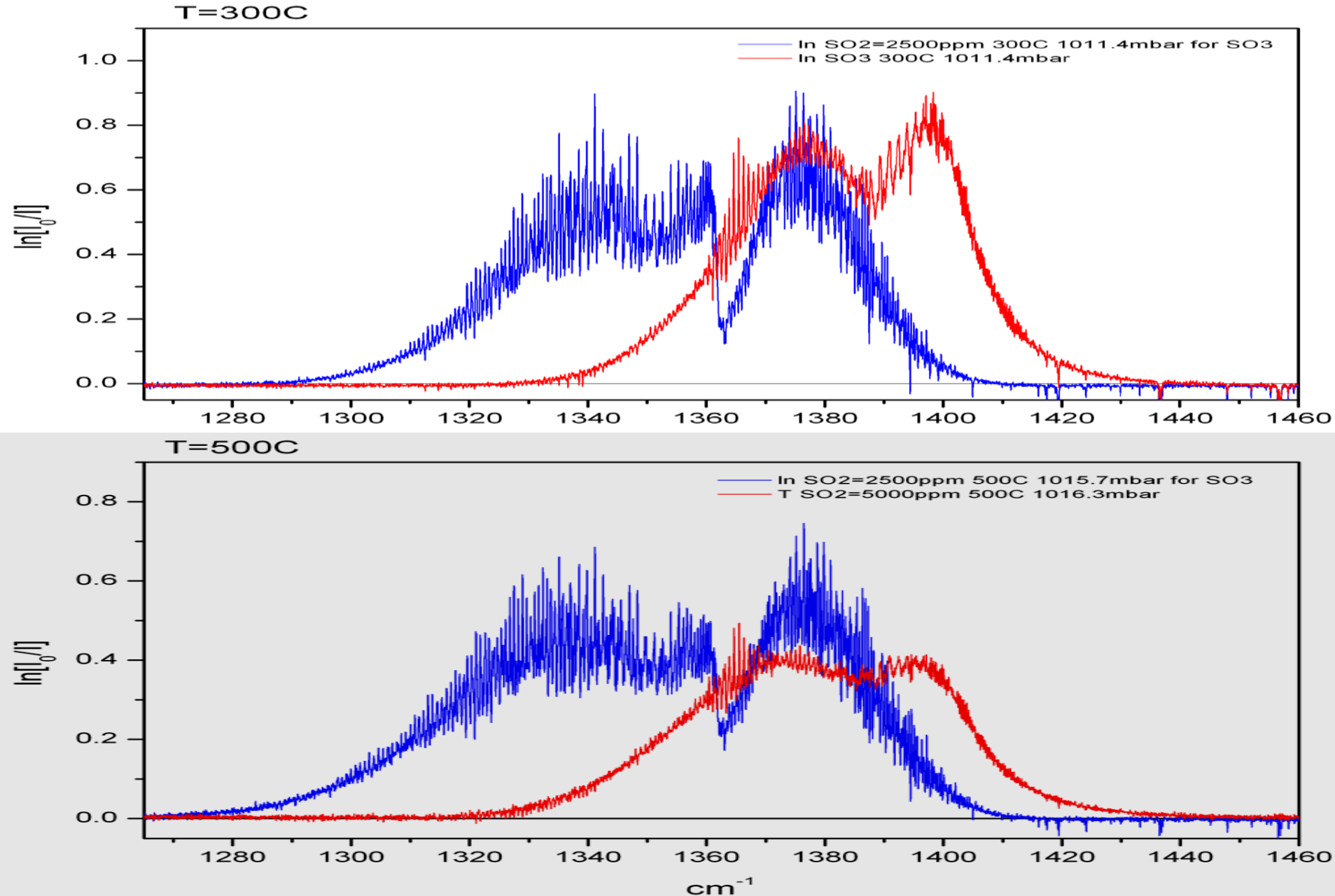
Challenges of the project:

- temperature range 200-500C;
- SO3 high-resolution spectra (SO3 generation);
- SO2, NH3, H2SO4 and H2O high-resolution spectra database;
- water cooled optical probe development;
- powerful IR light source development;
- high sensitivity FTIR with linearized MCT or InSb detector;
- use of modern mathematical tools (e.g. SVD, NNLS).

Two phases of the project:

- measurements in the lab and SO2/SO3 line list generation (UCL, UK)
- measurements on an industrial scale (power plant, Dong Energy, DK)

SO3 project: high-resolution (0.115 cm⁻¹) measurements



Conclusions

High quality optical measurements with various gases (incl. highly corrosive gases) are possible;

A new gas cell is under development (<200 bar, 2000°C)

Measurements can be used for: databases development and validation, studies of chemical reactions, energy exchange, validation of line shape models.

SO₃ project is under development: lab work + PhD student employed by UCL;

Trace gases in gasification project is under development: lab work + PhD student employed by DTU



Acknowledgements

- Energinet.dk: projects No. 2010-1-10622, 2010-1-10422
- Dong Energy
- UCL (Prof. Jonathan Tennyson)